LA-UR-15-27772

Diagnostic Needs for the Matter-Radiation Interactions in Extremes (MaRIE) Project

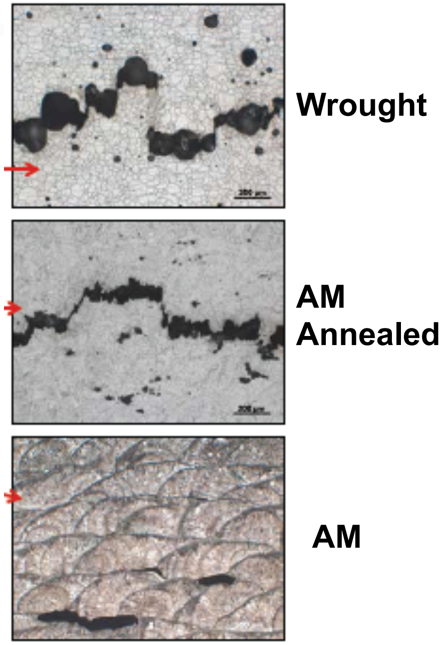
Cris W. Barnes, Michael F. Stevens,
Zhehui “Jeff” Wang, LANL

October 7, 2015

UNCLASSIFIED

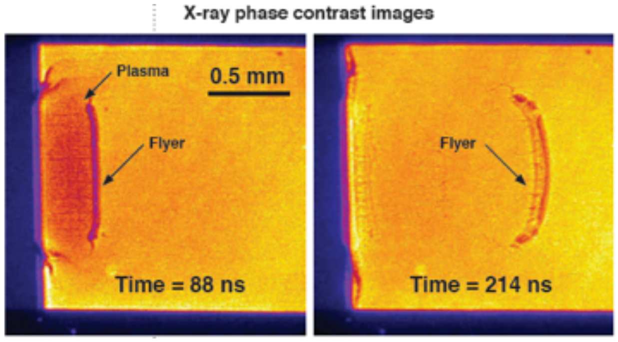
MaRIE will address the control of performance and production of weapons materials at the mesoscale

Performance of additively-manufactured structural components



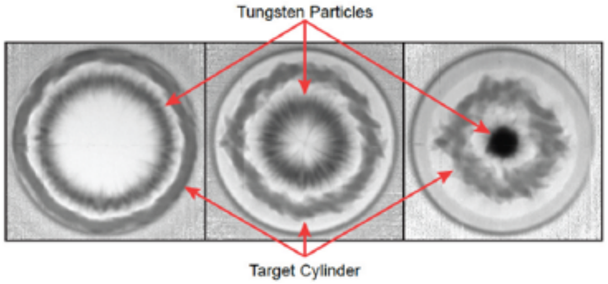
Damage in wrought vs additively-manufactured steel

Detonator performance and safety in LEPs



Movies of exploding bridge wire detonators

Ejecta and Mix in aged components under re-use

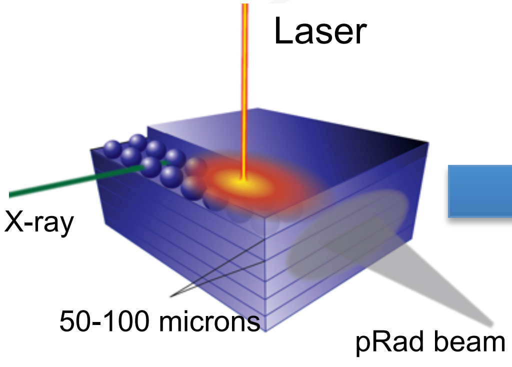


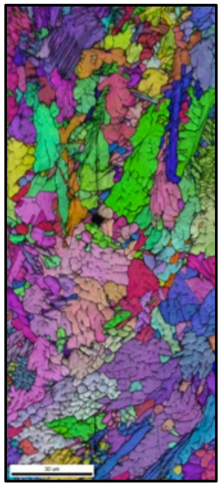
Movies of ejecta in convergent geometry

Requirements for MaRIE are set from analysis of such experiments.
--*"(U) MaRIE First Campaigns," LA-CP-15-00501, June, 2015*

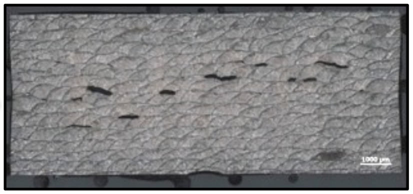
MaRIE fills a critical gap in length scale between the integral scale addressed by DARHT and U1a and facilities such as NIF and Z.

MaRIE will provide critical data to inform and validate advanced modeling and simulation to accelerate qualification of advanced manufacturing – move from “process-” to “product-based”



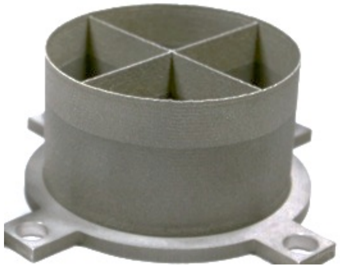


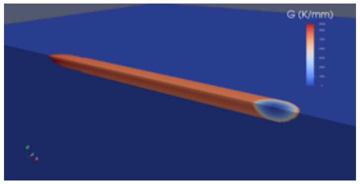
Additively Manufactured 316L Stainless Steel



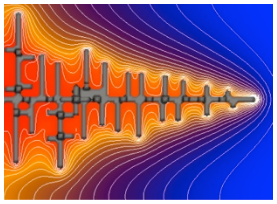
Damage under shock loading unable to coalesce leading to a tougher, more shock resistant material

Prototype Gas Bottle

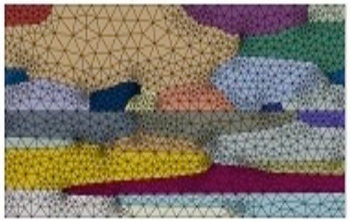




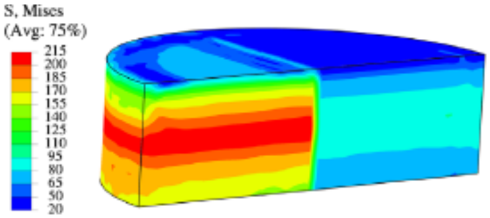
Process Modeling



Microstructure Modeling



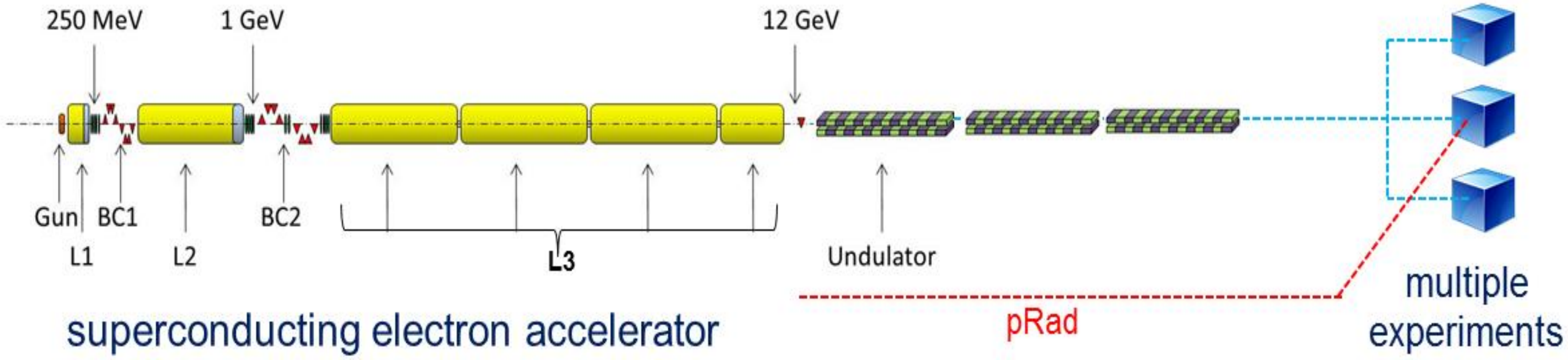
Properties Modeling



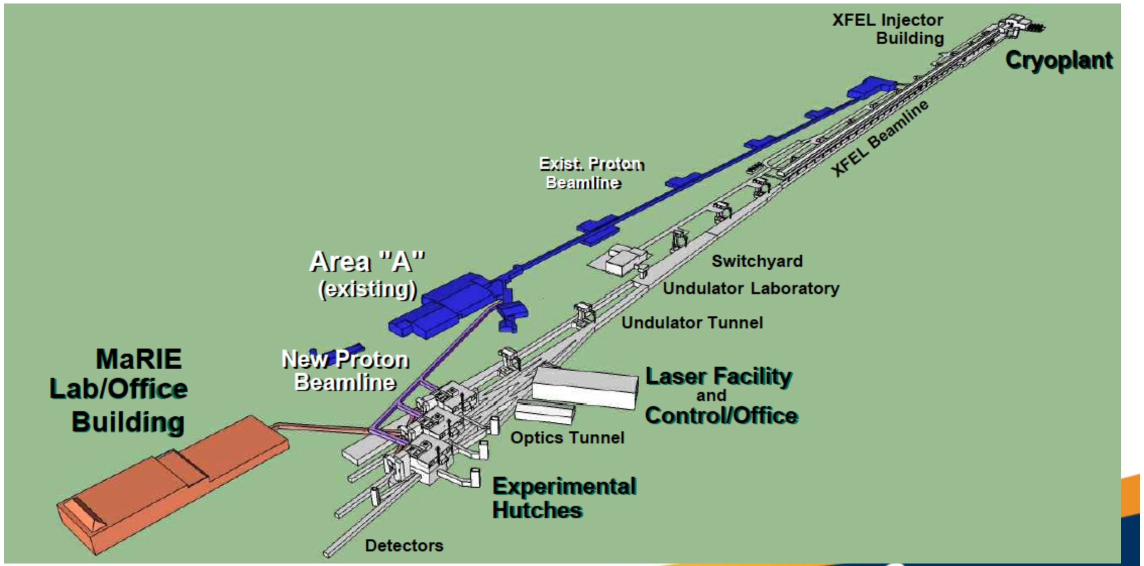
Performance Modeling

MaRIE and Exascale will enable rapid and confident deployment of new concepts and components through more cost-effective and more rigorous science-based approaches.

MaRIE (the Project) would provide this capability by building a 12-GeV electron linac feeding a 42-keV XFEL with experimental facilities

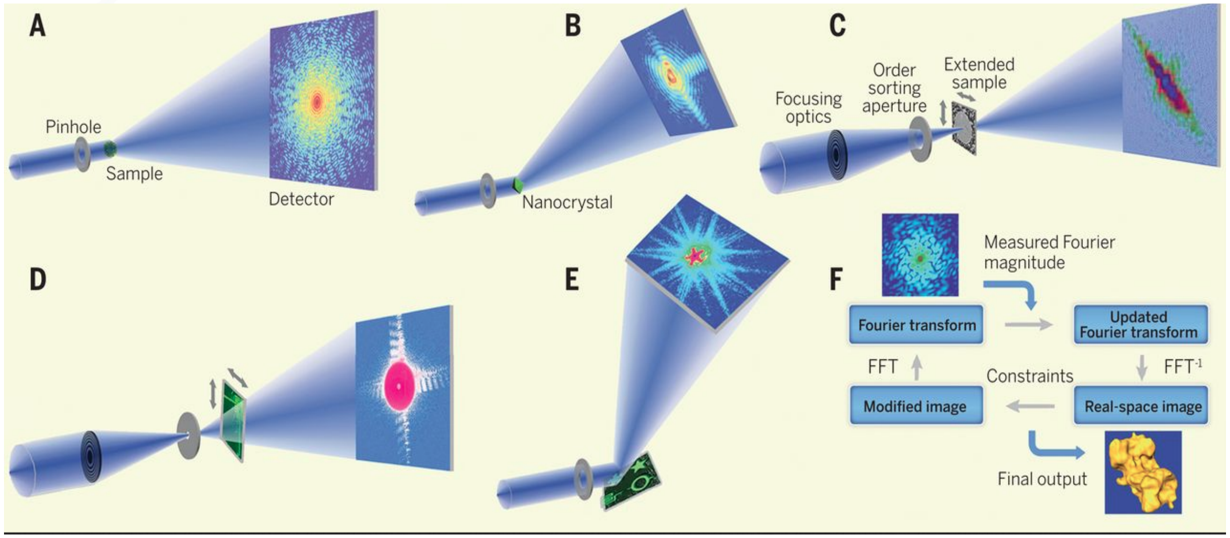


Our pre-conceptual reference design would be located on the north side of the LANSCE mesa, leveraging the capabilities of that proton/neutron facility.

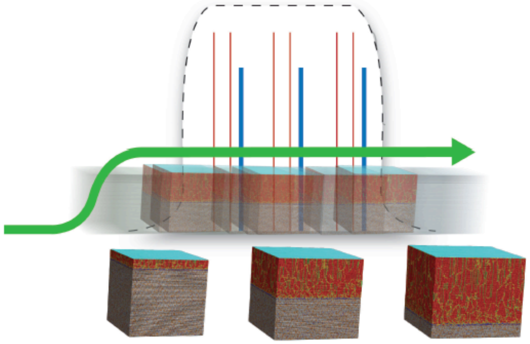


To see with time-dependence into and through the mesoscale requires: x-rays; coherent; brilliant and high repetition-rate; of sufficient high energy; and multiple probes at multiple scales

MaRIE builds on the major technical revolutions in: **x-ray lasers** and their brilliance (for time-dependence); and **coherent imaging** (allowing high-resolution observation of non-periodic microstructure).



From “Beyond crystallography: Diffractive imaging using coherent x-ray light sources,” by J. Miao, T. Ishikawa, I. K. Robinson, and M. M. Murnane, *Science* **348** (1 May 2015), pg 530.



The concept features multiple probes (x rays, protons, electrons, optical photons) to maximize the science.

- **Harder in energy for mesoscale and high-Z materials**
- **Higher in repetition rate to make movies of microstructure evolution**
- **Multiple probes to support maximum science return**

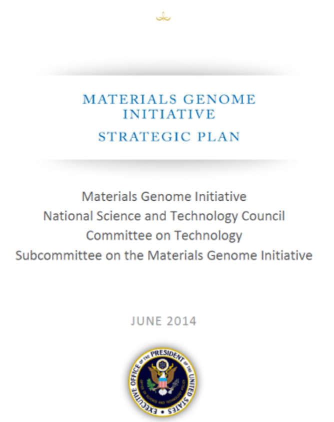
The motivated and justified capabilities from Defense Programs also address other national grand challenges

meso2012.com Materials Genome Advanced Manufacturing


SEPTEMBER 2012

FROM QUANTA TO THE CONTINUUM:
OPPORTUNITIES FOR MESOSCALE SCIENCE

A REPORT FOR THE BASIC ENERGY
SCIENCES ADVISORY COMMITTEE
MESOSCALE SCIENCE SUBCOMMITTEE


MATERIALS GENOME
INITIATIVE

STRATEGIC PLAN

Materials Genome Initiative
National Science and Technology Council
Committee on Technology
Subcommittee on the Materials Genome Initiative

JUNE 2014


REPORT TO THE PRESIDENT ON
ENSURING AMERICAN
LEADERSHIP IN ADVANCED
MANUFACTURING

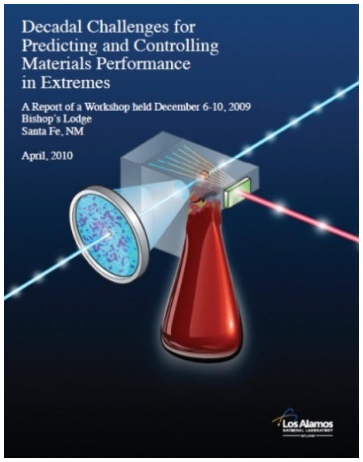
Executive Office of the President
President's Council of Advisors
on Science and Technology

science.energy.gov

Whitehouse.gov

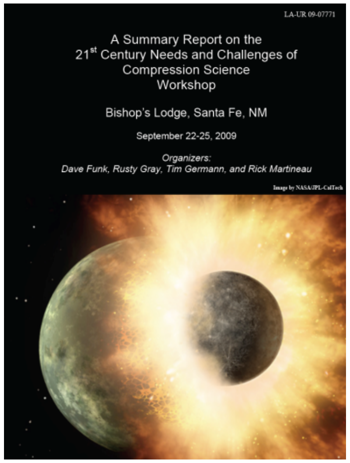
"Seizing this key opportunity requires mastering the mesoscale, where classical, quantum, and nanoscale science meet. It has become clear that in many important areas the functionality that is critical to macroscopic behavior begins to manifest itself not at the atomic or nanoscale but at the mesoscale, where defects, interfaces, and non-equilibrium structures are the norm."

BESAC "Opportunities in Mesoscale Science," 2012.


Decadal Challenges for
Predicting and Controlling
Materials Performance
in Extremes

A Report of a Workshop held December 6-10, 2009
Bishop's Lodge
Santa Fe, NM

April, 2010


LA-UR 09-07771

A Summary Report on the
21st Century Needs and Challenges of
Compression Science
Workshop

Bishop's Lodge, Santa Fe, NM

September 22-25, 2009

Organizers:
Dave Funk, Rusty Gray, Tim Germann, and Rick Martineau

Image by NASA/JPL-CalTech

"In closing I should note that in addition to critical NNSA programmatic needs, the MaRIE experimental capability will address basic science issues of mesoscale functionality of materials that is at the very forefront of basic energy sciences today. As such, this facility, if built, will certainly be applicable to some of the most important fundamental issues of how we can create new materials with controlled functionality."

John C. Hemminger

UNCLASSIFIED

The Matter-Radiation Interactions in Extremes (MaRIE) project has followed a rigorous pre-conceptual approach to meet mission and science challenges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SEPTEMBER 2012

FROM QUANTA TO THE CONTINUUM: OPPORTUNITIES FOR MESOSCALE SCIENCE

A REPORT FOR THE BASIC ENERGY SCIENCES ADVISORY COMMITTEE MESOSCALE SCIENCE SUBCOMMITTEE

REPORT TO THE PRESIDENT ON ENSURING AMERICAN LEADERSHIP IN ADVANCED MANUFACTURING

Executive Office of the President
President's Council of Advisors on Science and Technology

- **Lead and participate in scientific community <u>Workshops</u> and studies surveying the decadal challenges for materials science**
- **<u>Motivate</u> the science need for the mission through development of “First Campaigns”***
- **Develop and <u>Justify</u> the science functional requirements by analysis of detailed “First Experiments” in each mission-relevant campaign**
  - Conclude that a coherent, brilliant x-ray source that has energy and repetition rate characteristics matched to address materials performance challenges is required

Develop <u>pre-conceptual reference designs</u>, that can meet the requirements, with credible scope, cost and schedule estimates, and that can determine technical risks and define technology maturation plans

Dynamic Materials Performance

First Campaigns

Multiphase High Explosive Evolution

Dynamic Performance of Plutonium and Surrogate Metal Alloys

Turbulent Material Mixing in Variable Density Flows

Process-Aware Manufacturing

First Campaigns

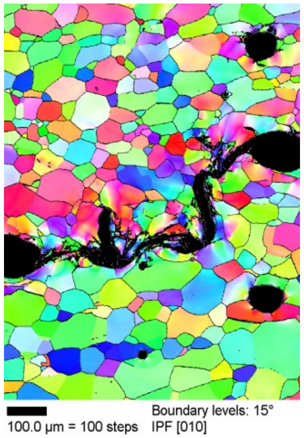
Old Materials: Aging

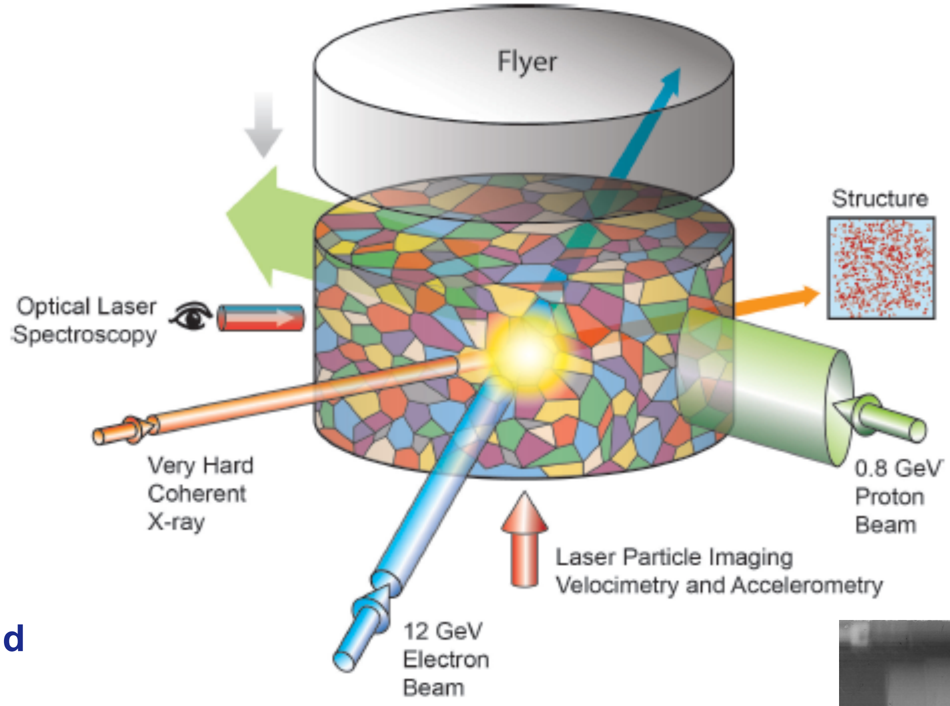
New Materials: Controlled Functionality

New Processes: Advanced and Additive Manufacturing

*“(U) MaRIE First Campaigns,” LA-CP-15-00501

The challenge is to observe the dynamic microstructure and phase evolution in materials down to the sub-granular level while connecting to the macroscale





Requirements:
Sub-μm space resolution
100's – 1000's-μm samples
Sub-ns time resolution,
~30 frames in
1−10-μs duration

The model:

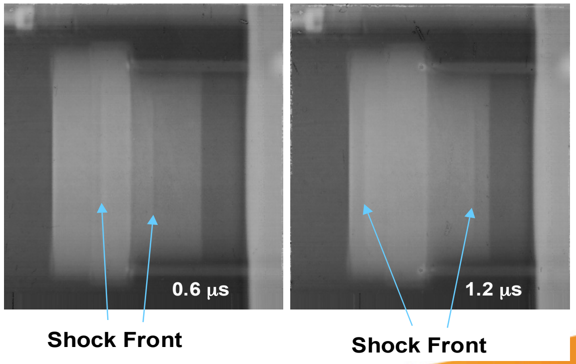
Accurate sub-grain models of microstructure evolution coupled to molecular dynamics

The goal

Predict dynamic microstructure and damage evolution

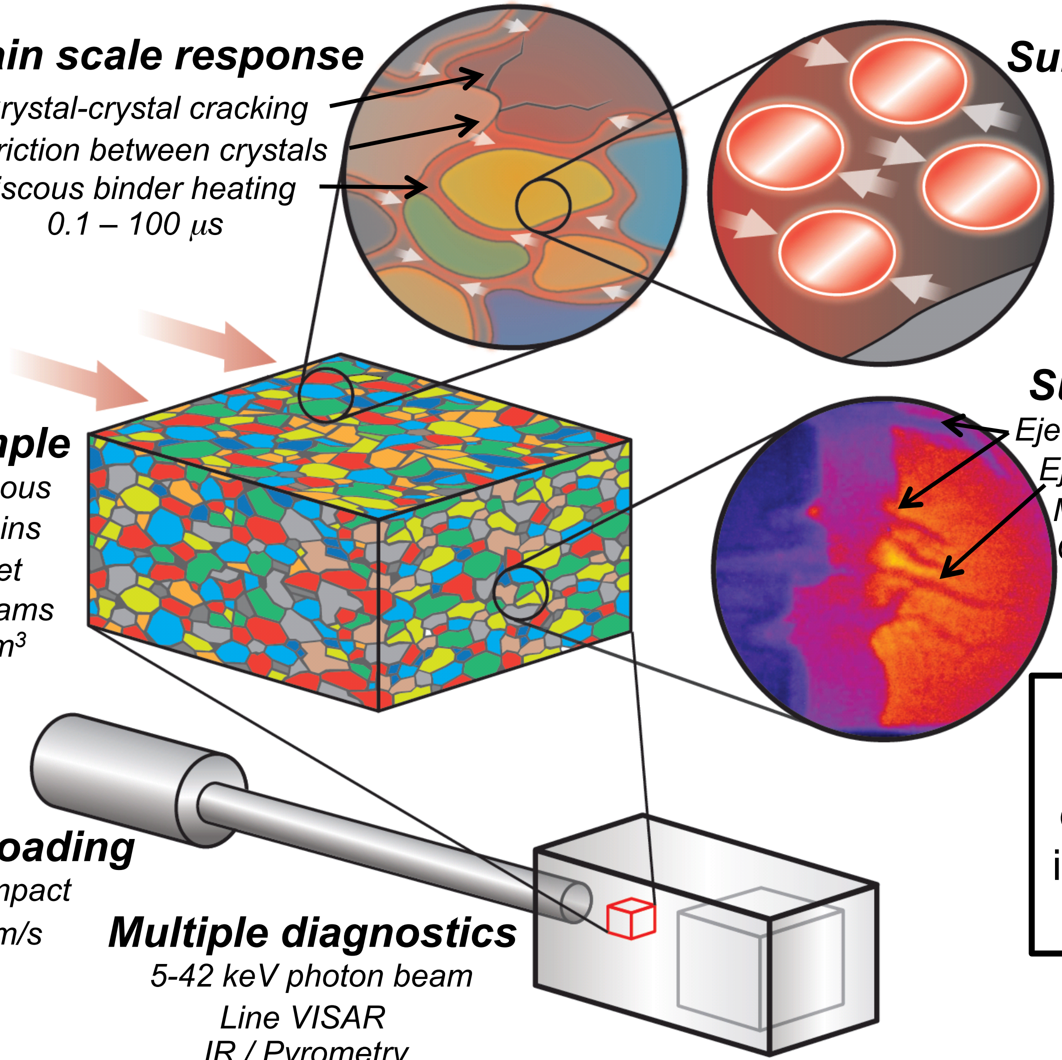
The first experiment

Multiple, simultaneous dynamic *in situ* diagnostics with resolution at the scale of nucleation sites (< 1 μm; ps – ns)



MaRIE allows us to break apart the problem

MaRIE allows *in situ* study of hot spot formation and other microstructural phenomena



Grain scale response

Crystal-crystal cracking
Friction between crystals
Viscous binder heating
0.1 – 100 μs

Sub-grain response

Void collapse
Localized heating
Phase transformation
10 – 1000 ns

Surface response

Ejecta from machining defects
Ejecta from cracks
Material strength
Complex shock interactions
10 – 1000 ns

PBX sample

Heterogeneous
Multiple grains
Prill or pellet
1 – 1000 grams
0.5 – 500 cm^3

Gas gun loading

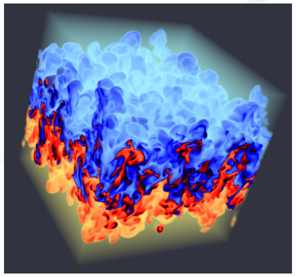
Projectile impact
0.05 – 5 km/s

Multiple diagnostics

5-42 keV photon beam
Line VISAR
IR / Pyrometry

MaRIE will directly observe hot spot formation and mesoscale deformation mechanisms within insensitive PBX materials during dynamic loading.

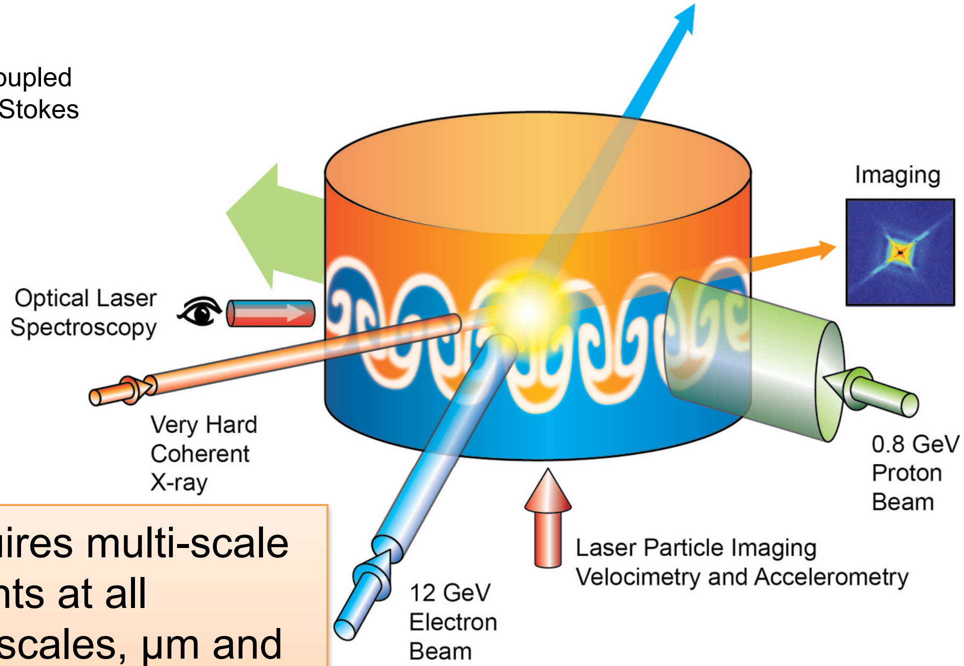
In situ and simultaneous measurement of turbulence and mixing at multiple length and time scales

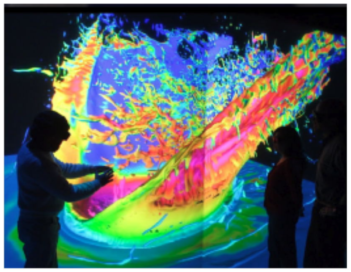


Direct Numerical Simulation coupled to Reynolds-Averaged Navier Stokes turbulence model

Material Samples:
Z values: from Be to Pu
“Two-dimensional” 0.05-0.5-mm thick, 1-5 mm in the shock direction, 3-15 mm in the thick direction

Measurements in Dynamic Environment:
3D imaging with 1 μm resolution
Phase within a grain
Density: 1%, in both directions transverse to the shock front with 1 μm (thin direction) or 10 μm (thick) and <10-ps resolution;

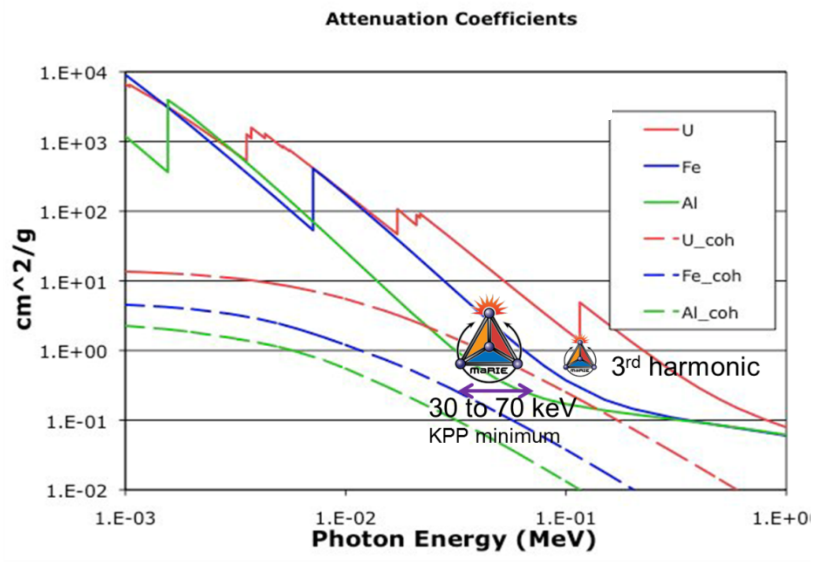




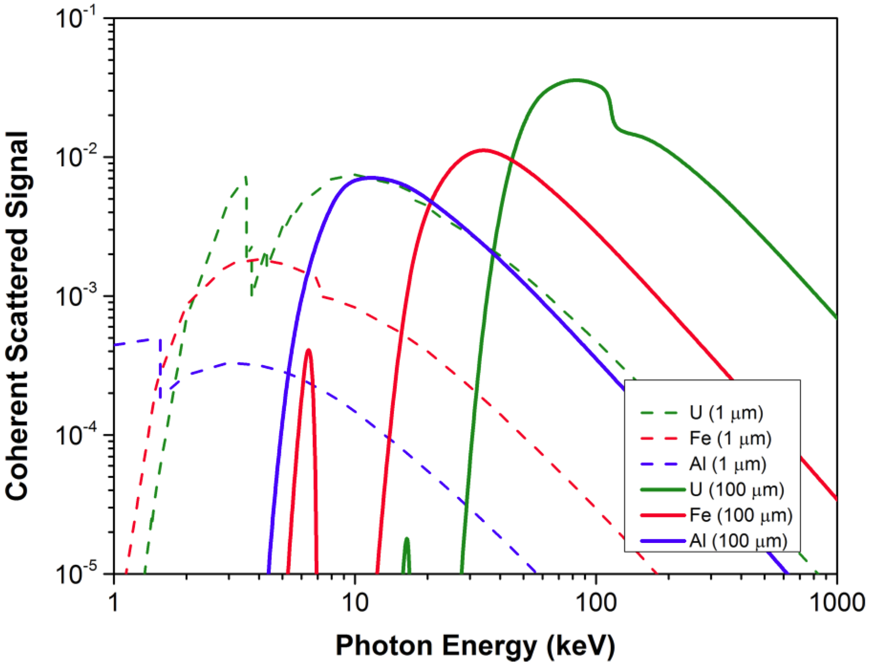
Develop predictive capability for turbulent mix

Predictive capability requires multi-scale fluid dynamics experiments at all relevant space and time scales, μm and μsec, with opaque materials and/or high-velocity flows requiring high repetition measurements.

The 42-keV energy of the reference design is a trade-off between maximizing elastic scattering for diffraction, minimizing absorptive heating, and sample thickness in plutonium – other elements are easier.



A high resolution image requires a minimum number of coherently scattered photons per sub-ps pulse. This sets the incident number of photons on a sample of ~$2x10^{10}$.



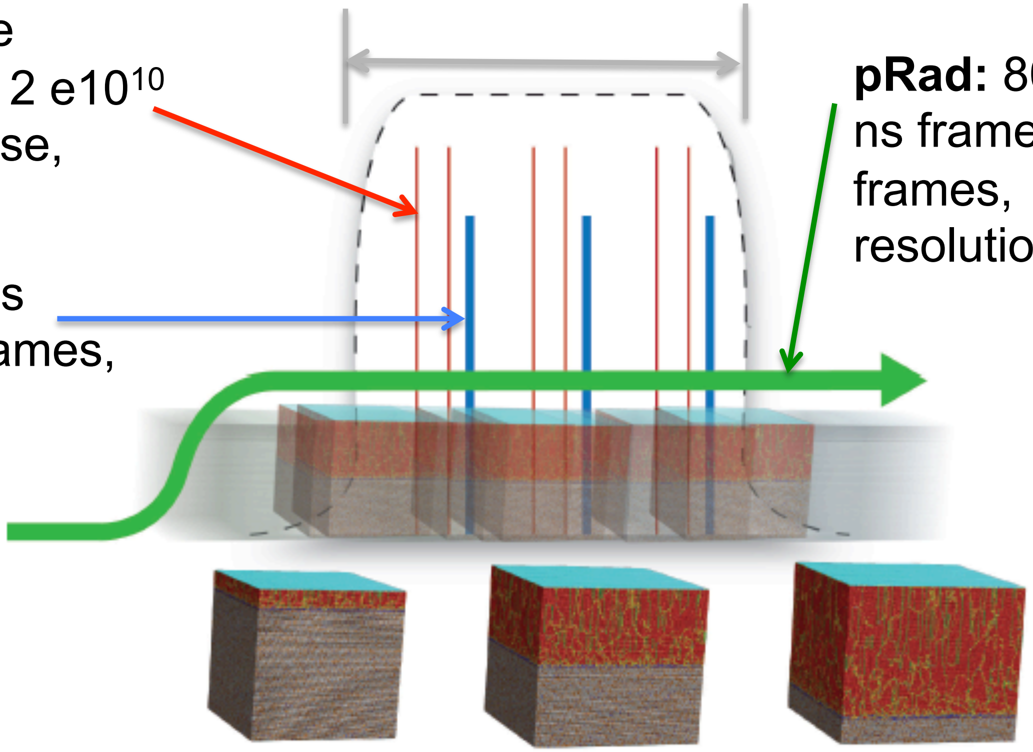
The fraction of incident photons coherently scattered just once, the coherent scattering signal, as a function of incident photon energy for various materials at thicknesses of 1 *μ*m (dashed lines) and 100 *μ*m (solid lines)

J. L. Barber *et al.,* Phys. Rev. B **89** (2014) 184105

MPDH multiplexes 42-keV x-ray photons (red), 12-GeV electrons (blue), and 0.8-GeV protons (green) to interrogate a single dynamic event to support maximum science return

XFEL: 42 – 126 keV (3Ω); 300 ps frame speed, 30 frames, 2 e10^{10} photons@50fs/pulse, >0.1μm resolution

eRad: 12Gev, 25 ns frame speed, 30 frames, >1 μm resolution, 2 nC/pulse



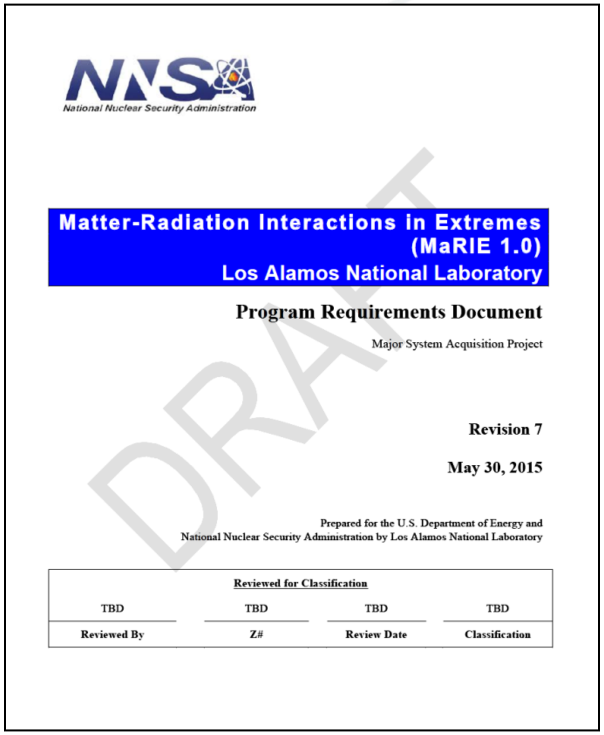
pRad: 800Mev, 5 – 50 ns frame speed, 30 frames, 20 – 30 μm resolution

Spatial and Temporal resolutions for MaRIE 1.0 mesoscale experiments are defined by analysis of the measurement techniques

	Metals Manufacture and Age aware performance	**HE certification and qualification**	**Turbulent Materials Mixing**	**Welding and Additive Manufacturing**
resolution	100 nm - 20 µm	100 nm - 20 µm	500 nm	1 µm – 100 µm
Field of View	100 µm - 1 mm	100 µm - 2 mm	1 mm	0.3 mm – 1 cm
# of frames	up to 30	up to 30	up to 30	1000 per second
min pulse sep	300 psec	500 psec	30 nsec	10 nsec
macropulse length	10 µsec	7 µsec	15 µsec	100 µsec
sample thickness	> 250 µm	> 10 µm – 6 cm	1 – 10 cm	0.1 to 10 mm
species	Be - Pu	Typically C, H, O, N	Noble gases, Ga, Be	Be - Pu

	spatial resolution	**Framing time**	**sample thickness# Z=13**	**sample thickness# Z=26**	**sample thickness# Z=92**
prad*	> 20 µm	50 nsec	15 cm / 0.8 GeV	3 cm / 0.8 GeV	1 cm / 0.8 GeV
erad*	> 1 µm	> 25 nsec	6 cm / 12 GeV	5 mm / 12 GeV	1 mm / 12 GeV
X ray	> 0.1 µm	< 100 psec	>10 µm/ 8 keV 2 cm/ 42 keV	500 µm/42 KeV 4 mm/122 KeV	200 µm/42 KeV 2 mm/122 KeV

The Key Performance Parameters proposed in the Program Requirements Document quantify the requirements



National Nuclear Security Administration

Matter-Radiation Interactions in Extremes (MaRIE 1.0)
Los Alamos National Laboratory

Program Requirements Document

Major System Acquisition Project

Revision 7

May 30, 2015

Prepared for the U.S. Department of Energy and
National Nuclear Security Administration by Los Alamos National Laboratory

Reviewed for Classification

TBD	TBD	TBD	TBD
Reviewed By	**Z#**	**Review Date**	**Classification**

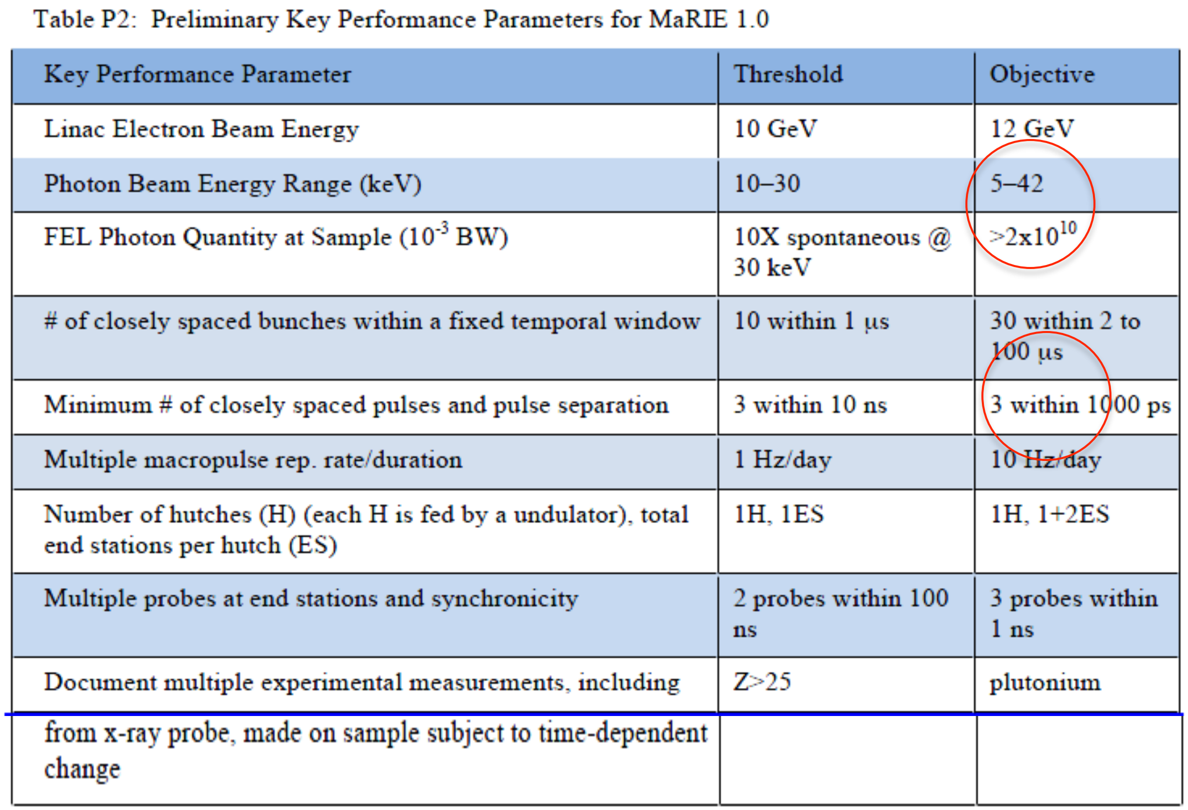
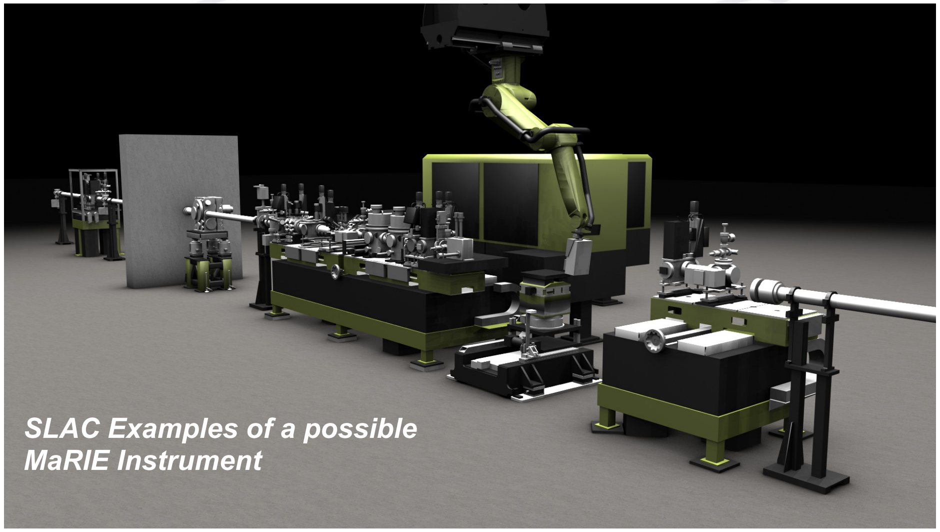


Table P2: Preliminary Key Performance Parameters for MaRIE 1.0

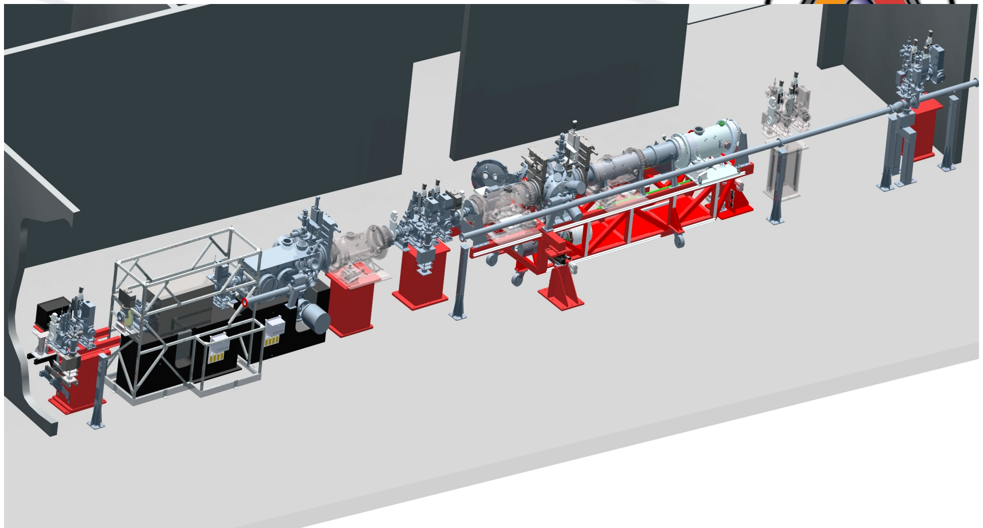
Key Performance Parameter	Threshold	Objective
Linac Electron Beam Energy	10 GeV	12 GeV
Photon Beam Energy Range (keV)	10–30	5–42
FEL Photon Quantity at Sample (10^{-3} BW)	10X spontaneous @ 30 keV	$>2x10^{10}$
# of closely spaced bunches within a fixed temporal window	10 within 1 μs	30 within 2 to 100 μs
Minimum # of closely spaced pulses and pulse separation	3 within 10 ns	3 within 1000 ps
Multiple macropulse rep. rate/duration	1 Hz/day	10 Hz/day
Number of hutches (H) (each H is fed by a undulator), total end stations per hutch (ES)	1H, 1ES	1H, 1+2ES
Multiple probes at end stations and synchronicity	2 probes within 100 ns	3 probes within 1 ns
Document multiple experimental measurements, including from x-ray probe, made on sample subject to time-dependent change	Z>25	plutonium

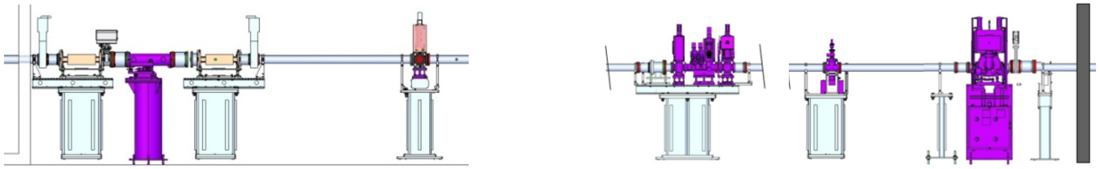
Further detailed scientific requirements have been motivated and justified – but will be revisited in a series of user community workshops after CD-0.

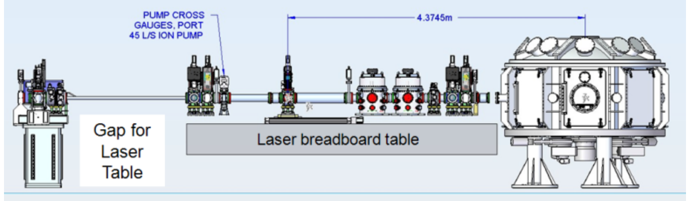
Experimental Facilities Equipment is based on Existing Hardware at LANL, SLAC, and ANL with planned improvements through R&D

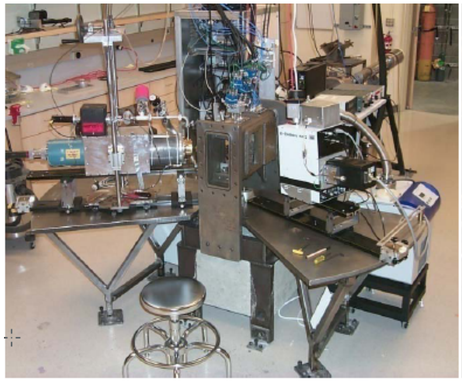


SLAC Examples of a possible MaRIE Instrument

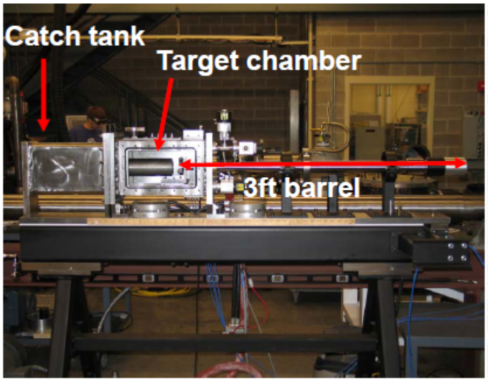






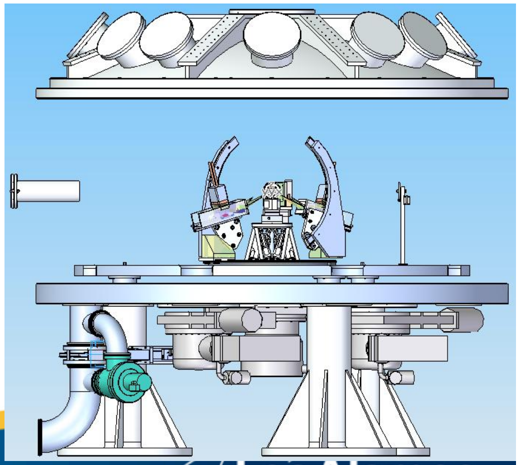


XRD Powder Gun

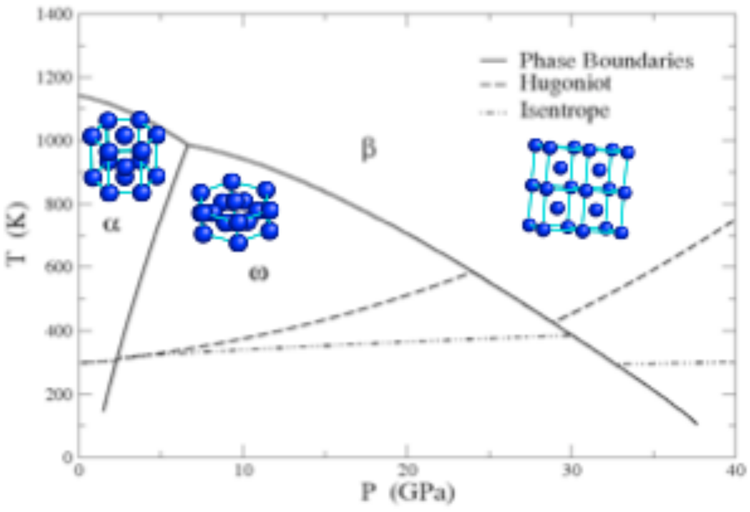


Gun used at APS

Pulser

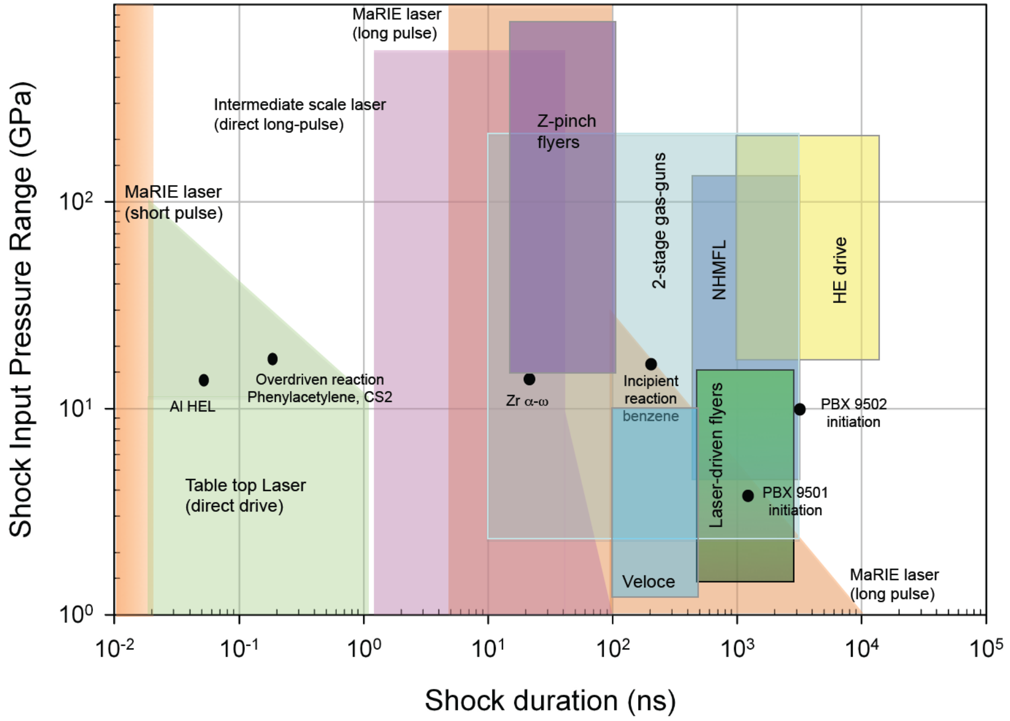


Drivers for dynamic environments focus on rich regime <200 GPa and shock durations relevant to the mesoscale

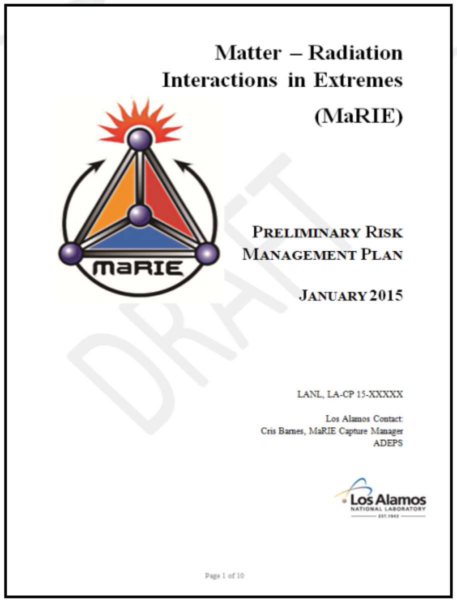


Zr P-T phase diagram

(courtesy of C. Greeff, LANL, Modelling Simul. Mater. Sci. Eng. 13, 1015)



Technology Maturation Plans to mitigate high-consequence technical risks have been identified



Matter – Radiation
Interactions in Extremes
(MaRIE)

PRELIMINARY RISK
MANAGEMENT PLAN

JANUARY 2015

LANL, LA-CP 15-XXXXX

Los Alamos Contact:
Cris Barnes, MaRIE Capture Manager
ADEPS

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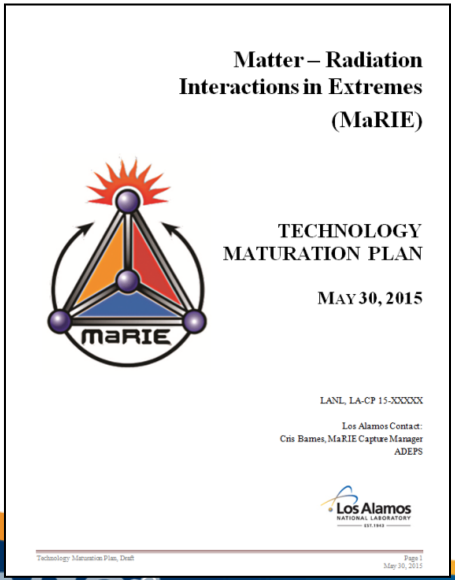


Matter – Radiation
Interactions in Extremes
(MaRIE)

TECHNOLOGY
MATURATION PLAN

MAY 30, 2015

LANL, LA-CP 15-XXXXX

Los Alamos Contact:
Cris Barnes, MaRIE Capture Manager
ADEPS

Technology Maturation Plan, Draft

Page 1
May 30, 2015

Subsystem or Component	Risk Events	Consequences	Representative TRL
XFEL Linac	Beam emittance requirements not met; Wakefields last longer in time than predicted; Beam energy spread requirements not met; Insufficient photon flux in the required bandwidth	1) Inability to meet $2x10^{10}$, 42-keV within $2x10^{-4}$ bandwidth requirement for single shot CDI imaging. 2) Minimum x-ray pulse separation more than 300 ps not allowing framing rates that capture short duration events.	2
Detectors	Small pixel sizes, sub-ns framing times, fast on-board storage, good quantum efficiency, low noise, high dynamic range detectors not feasible or affordable; staff expertise not available in time for project construction	The X-ray source cannot be used efficiently to generate sufficient data for the image construction and code validation; Long stand-off distances increase conventional facility costs, reduce resolution; more detectors and imaging stations required; resolution requirements not met; devices not available when required for experimentation	2
Combined X-ray/pRad for quasi-3D experimental	New image analysis techniques unsuccessful	Cannot obtain quasi-3D information on dynamically loaded samples at > 1 keV x-ray energies	1

As a diagnostic example, consider the challenges of fast, repetitive hard x-ray detection

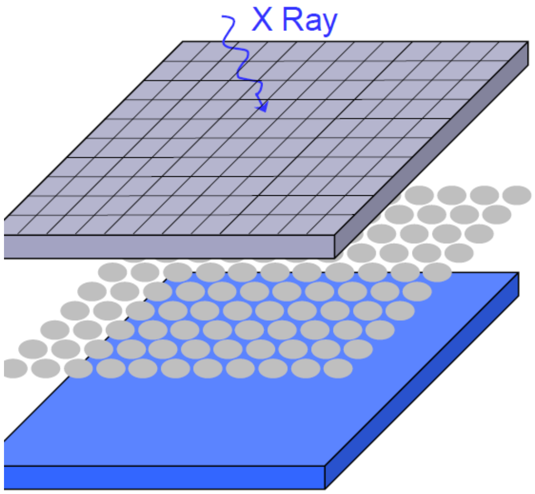
- The picosecond challenge: high efficiency (>50%) x-ray detection with fast gating.
- The GigaHertz challenge: time resolution / framing for acoustic velocities across grains
- The TerraByte challenge: dealing with possible big data sets to inform scientific "co-design"

Comparison with ICF/HED requirements

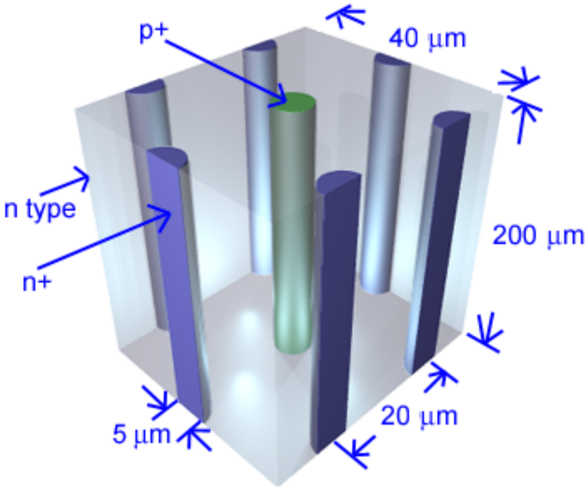
Parameters	**ICF/HED**	**“MaRIE camera”**
X-ray Source coherence	No	Yes
Spectral range (keV)	<10	5 to > 42 keV
Frame rate (GHz)	1-1000	3-10
Dynamic range	1-10^2 ph	1-10^3 ph (14-bit)
QE @ 15 keV	> 80%	> 90%
QE @ 42 keV	<5%	> 50%
QE @ 126 keV	<2%[5]	> 50%
In-pixel memory	10-100	10 - 100
Pixel pitch	< 10 μm	> 25 μm
Number of pixels	1024^2	128^2 to 1024^2
Sensor thickness (μm)	< 500	~ 1000 or more

Possible MaRIE Camera Concepts (direct detection)

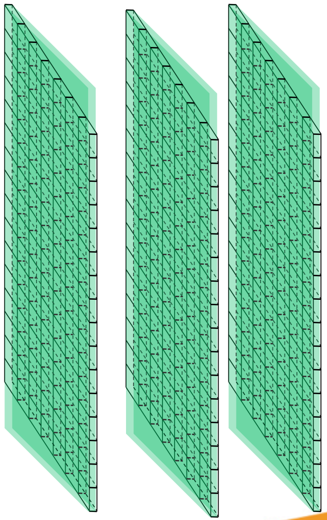
- **High-Z Hybrid**
  - ~42 keV
  - Room temp.
  - GaAs:Cr
  - 50 MHz ASIC
- **3D silicon Hybrid**
  - Integration
  - ~ 42 keV
  - GHz ASIC
- **Multilayer monolithic**
  - C (diamond), Si
  - 42 - 126 keV
  - New design; ~one x-ray per layer
  - GHz ASIC



Tomsk U.



R. Bates



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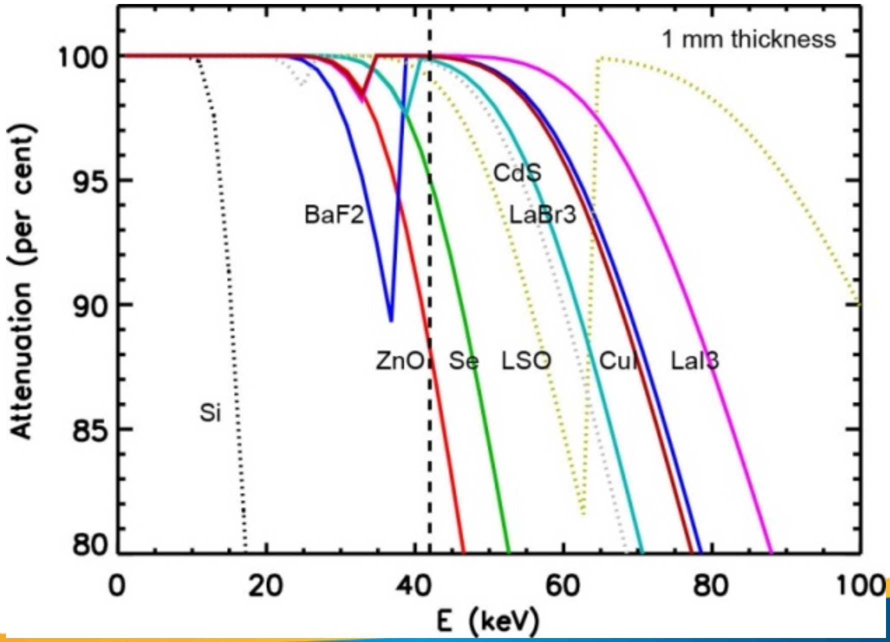
There are concepts for “indirect” detection possible for development

- **Fast scintillators**
  - Materials (BaF_2)
  - Structure (photonic crystals
  - Fast, efficient photodetectors
- **Wide bandgap semiconductors**
  - ZnO?
  - GaN
  - Fabrication issues
- **Nano things**
  - Quantum dots
  - Nanowires



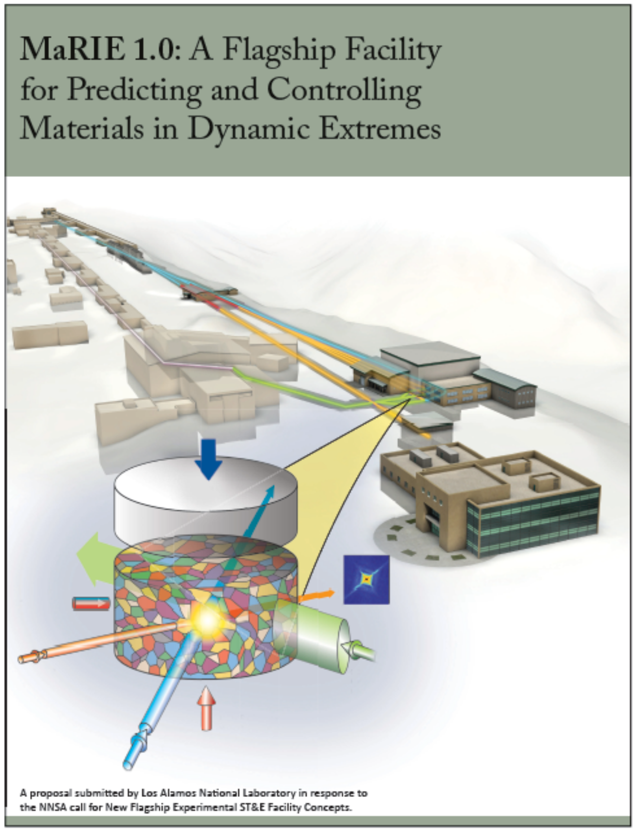
Z. Wang (2013)

Technology Maturation for a MaRIE x-ray detector will establish parallel concept development each following four tasks

- **Task 1: Architecture & Design**
  - To select a detector architecture (2D, 3D) and sensor material use
  - fast ASIC
- **Task 2: Fabrication**
  - To demonstrate scalable prototypes
    - 16 x 16 prototype efficiency or frame-rate by year 4
    - 16 x 16 prototype efficiency *and* frame-rate by year 7.
  - To come up with a fabrication plan/procedure
- **Task 3: Testing**
  - To validate the design and fabrication through measurements
- **Task 4: Collaboration and coordination**
  - Team building
  - To coordinate different activities

A Vision: Use the MaRIE detector "application" to connect to advanced materials scientists to drive new detector concepts.

MaRIE 1.0 will enable us to observe and ultimately control the time-dependent properties of materials that affect materials performance and production



MaRIE 1.0: A Flagship Facility for Predicting and Controlling Materials in Dynamic Extremes

A proposal submitted by Los Alamos National Laboratory in response to the NNSA call for New Flagship Experimental ST&E Facility Concepts.

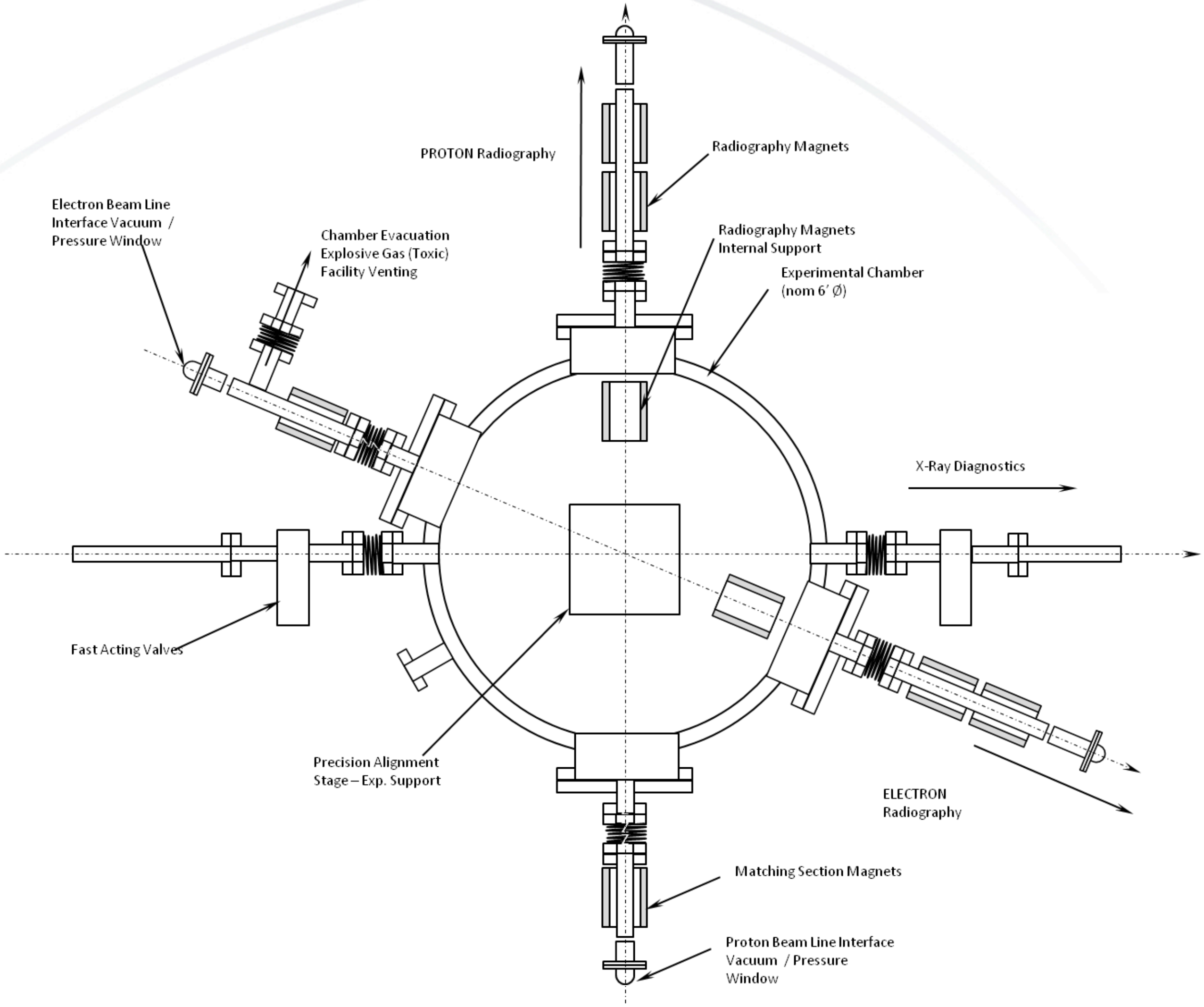
A mission need exists for a facility focused on predicting and controlling materials in extreme environments, exploiting *in situ* transient measurements with an XFEL on real materials in relevant dynamic extremes to **address national security challenges in qualification, certification, and assessment**.

Achieving controlled functionality at the mesoscale through co-design is the **frontier of materials research** and requires an advanced experimental facility.

MaRIE 1.0 meets this need with a robust preconceptual reference design that is grounded in **community-defined mission and scientific requirements**.

BACKUP

MPDH Test Chamber Schematic



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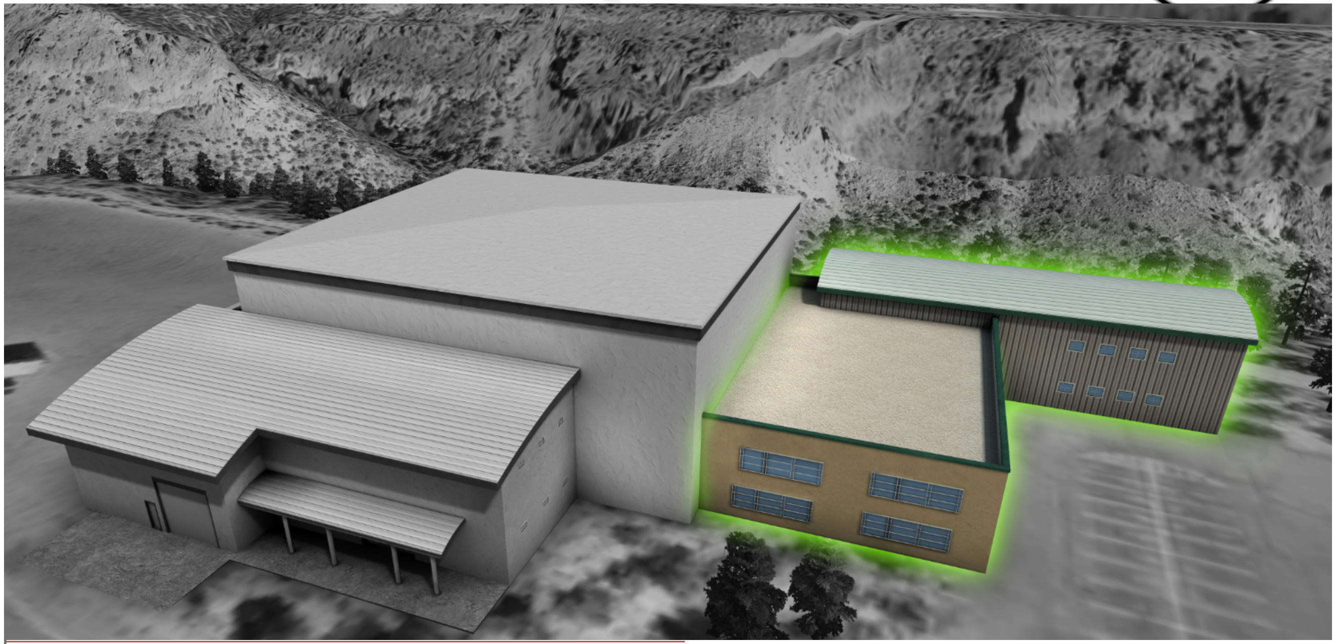
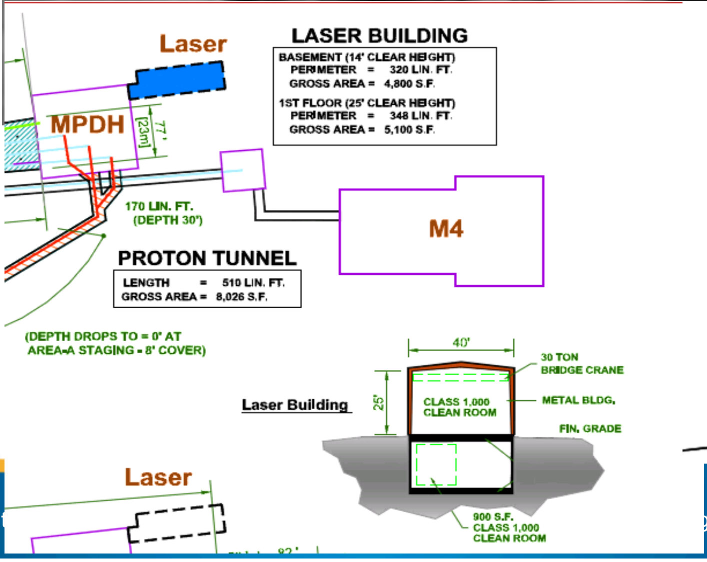
MPDH Laser Facility – Scope during Proposal Submission

MPDH Laser Facility & Support Building

- Includes laser hall @ 40' x 140’ two story pre-engineered building 25’ clearance total 5,100 SF.
- Basement with 12” concrete walls and 30” concrete slabs for floor and ceiling total 4,800 SF.
- Class 1000 Clean room 1st floor and Class 1000 Clean Room in basement.
- Drywall around walls and ceiling with epoxy coating on all surfaces 1st floor.
- Wet Pipe Sprinkler System with 6” Riser.
- 1000 amp Electrical Distribution System for building utilities.
- Estimate is for structure and building utilities only.
- 2’ x 4’ Pendant mount lighting, receptacles and switches.
- 30-ton bride crane in 1st floor and Loading Dock @ 1st floor.

16,900 SF





LASER BUILDING

BASEMENT (14' CLEAR HEIGHT)
PERIMETER = 320 LIN. FT.
GROSS AREA = 4,800 S.F.

1ST FLOOR (25' CLEAR HEIGHT)
PERIMETER = 348 LIN. FT.
GROSS AREA = 5,100 S.F.

PROTON TUNNEL

LENGTH = 510 LIN. FT.
GROSS AREA = 8,026 S.F.

Laser Building